ELabELN | Template Use Case White Paper

Mass Spectrometry Experiment Template

Structured Documentation for Bottom-Up TMT Proteomics — From Protein Extraction Through Search and Differential Abundance Analysis

APPLIES TO

- Academic and life sciences research laboratories
- Biotechnology and pharmaceutical R&D groups
- Proteomics and mass-spectrometry core facilities
- Analytical chemistry labs and contract research organizations (CROs)

RELEVANT COMPLIANCE & INTEGRITY FRAMEWORKS

- FDA 21 CFR Part 11 — Electronic records and signatures
- EU Annex 11 — Computerized systems in regulated environments
- GAMP 5 — Software validation for regulated industries
- NIH / NSF reproducibility and FAIR data-management requirements

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1. Executive Summary

A quantitative proteomics experiment is one of the longest, most collaborative workflows in the life sciences. A single TMT study passes through many hands — a postdoc lyses and digests the samples, a facility scientist labels and runs them on the mass spectrometer, and a computational analyst searches and interprets the data — and through several external tools, from the Orbitrap's acquisition software to MaxQuant to Perseus. Every stage adds parameters that determine the result: which sample went in which TMT channel, the digest ratio, the fractionation, the LC gradient, the instrument resolution, the search database, the FDR threshold, and whether TMT ratio compression was corrected. When that chain lives across a shared spreadsheet, an instrument PC, and three people's memories, the study becomes impossible to reproduce and hard to trust — and the labeling scheme, the one thing that maps a fold change back to a sample, is the easiest of all to lose.

The ELabELN Mass Spectrometry Experiment Template solves this by providing a pre-built, fully structured run record that loads from the template library in a single click. It ships with a 10-step bottom-up TMT protocol, validated labeling and digest references, pre-wired instrument and search-engine parameters, and typed inputs for channel assignment, protein input, fractionation, LC gradient, MS acquisition mode, search database, and result-filtering thresholds. TMT reagents, trypsin lots, and columns link to the ELabELN inventory, and the tamper-evident audit trail captures every labeling scheme, every search-parameter set, and every analysis run.

This white paper describes what the template contains, the proteomics use case it is designed to support, the upstream and downstream workflows it connects to, the benefits it delivers to the team, and how a laboratory can deploy it and begin running cohorts within days.

> **KEY BENEFIT**
> Labs that adopt the MS template stop restating the method every run and losing the labeling scheme between hands, capture TMT-lot, column-life, and parameter provenance automatically across the whole pipeline, and gain a queryable, cross-cohort record — one place that ties every fold change back to its channel, its parameters, and the analyst who produced it.

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2. What Is Bottom-Up TMT Proteomics, and Why Does Documentation Matter?

2.1 The Technique

Bottom-up proteomics identifies and quantifies the proteins in a sample by digesting them into peptides, measuring the peptides by liquid chromatography–tandem mass spectrometry (LC-MS/MS), and matching the resulting spectra back to protein sequences. In a TMT (tandem mass tag) experiment, peptides from each sample are labeled with an isobaric tag carrying a distinct reporter ion, so that up to ten (or more) samples can be pooled and analyzed together, with relative abundance read from the reporter-ion intensities. The pooled sample is fractionated to reduce complexity, each fraction is separated on a nano-flow C18 column and fragmented in the mass spectrometer, and the data are searched against a protein database, filtered to a controlled false-discovery rate, normalized, and tested for differential abundance between groups.

This is the standard approach for quantitative proteomics, post-translational-modification mapping, biomarker discovery, and protein-interaction studies. Its power is depth and multiplexing; its difficulty is that the result depends on a long chain of choices made by different people using different software. TMT quantification in particular carries a well-known caveat — ratio compression, the underestimation of fold changes caused by co-isolated interfering precursors — whose handling (SPS-MS3 acquisition, or a correction applied at analysis) must be documented for the fold changes to be interpreted correctly.

Because a proteomics result is the product of many stages, many hands, and several tools, **the labeling scheme, the acquisition and search parameters, and the reagent lots are what make a study reproducible and comparable to the next cohort — which is exactly why they must live in one structured record rather than scattered across the people and machines that produced them.**

2.2 The Documentation Problem

Recording a proteomics run across spreadsheets, an instrument PC, and analysts' notes creates a set of interconnected risks:

- The TMT channel-to-sample assignment — the key that maps every quantitative result back to a sample — is kept in a spreadsheet that can be separated from the data, mislabeled, or lost.
- Instrument method, LC gradient, and acquisition mode are restated each run, so which parameters produced a given dataset is uncertain.
- Search engine, database version, and FDR threshold live with the analyst, disconnected from the sample prep and acquisition record.
- TMT reagent lot, trypsin lot, and column life are not captured against the run, so a batch effect cannot be traced to a reagent.
- Whether ratio-compression mitigation was applied is undocumented, so downstream fold changes are interpreted without the necessary caveat.
- Because the workflow spans several people, there is no single timestamped, attributed record of who did what — and prior cohorts cannot be retrieved to compare.

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These are the gaps that make proteomics studies hard to reproduce and compare, and they are the gaps this template was designed to close.

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3. Template Overview: What Ships with the Template

The ELabELN Mass Spectrometry Experiment Template is a pre-populated experiment record available to all ELabELN subscribers directly from the template library. It ships configured for a bottom-up TMT 10-plex proteomics study on cultured cell lysates, with a 10-step protocol covering protein extraction through MaxQuant search, normalization, and differential abundance analysis. The default configuration assumes a Thermo Q Exactive HF-X Orbitrap, TMT 10-plex isobaric labeling, an in-solution trypsin digest, high-pH reverse-phase offline fractionation into 12 fractions, online nano-LC separation on a 25 cm C18 column, and HCD fragmentation at NCE 32%, with each fraction analyzed in a separate 90-minute LC-MS/MS run. Every section is editable — the configuration is a tested baseline, not a locked format.

3.1 Template Sections at a Glance

The template populates the existing ELabELN experiment sections your lab already works in. Your team edits a working baseline instead of restating the method from scratch every run.

Section	What it pre-populates
Main Text	Study-design summary, instrument-method notes, and expected identification depth, authored in the TinyMCE rich-text editor and linked to the upstream lysate prep.
Extra Fields	Twelve structured, typed fields grouped as Sample, Labeling, and Acquisition — sample group, TMT channel assignment, protein input amount, digest enzyme and ratio, fractionation method, LC gradient, instrument and resolution settings, search engine and database, and FDR threshold. Typed values make labeling schemes and acquisition parameters queryable across cohorts.
Steps	A 10-step workflow checklist covering lysis through MaxQuant search and Perseus differential analysis. Each tick is timestamped to the audit trail, and the instrument run is auto-logged.
Compounds	TMT reagents, trypsin, the column, mobile phase, and reference protein digests pre-linked from the compound database, with the TMT lot shown inline with its channel and column-life tracked.
Links & Resources	Pre-wired to the lab's TMT 10-plex SOP v2.1, the UniProt human reference database, the instrument method file, and the Perseus workflow.
Storage & Files	−80 °C labeled-peptide aliquot storage, plus labelled attachment slots for raw .raw files, peptide.txt and proteinGroups.txt output, and Perseus session files.

Main Text
Study design summary, instrument method notes, expected ID depth.
Extra Fields
Typed: channel, group, input, digest, fractionation, LC, MS, search, FDR.
Steps
10-step checklist; each tick timestamped, instrument run logged.
Compounds
TMT reagents, trypsin, column, mobile phase, reference digests from inventory.
Links & Resources
TMT 10plex SOP v2.1, UniProt human, instrument method, Perseus workflow.
Storage & Files
−80 °C labeled-peptide aliquots; .raw, proteinGroups.txt, Perseus sessions.

Figure 1. The six ELabELN experiment sections pre-populated by the mass spectrometry template.

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3.2 The 10-Step Protocol

The workflow checklist is the operational spine of the template. Each step maps to a discrete bench, instrument, or computational action and writes a timestamped, user-attributed entry to the audit trail when checked off. The instrument run is auto-logged, and the search and differential-analysis steps are performed in external tools, with their parameters and results recorded as typed fields.

Step	Action	What it captures
1	Lyse & extract protein	Protein input amount
2	Digest (trypsin)	Digest enzyme and ratio
3	TMT label (10-plex)	Channel-to-sample assignment; TMT lot
4	Pool channels	Pooling
5	Fractionate (high-pH RP, 12)	Fractionation method
6	nano-LC-MS/MS (Orbitrap, HCD)	LC gradient; instrument & resolution (run auto-logged)
7	MaxQuant search	Search engine & database (external tool)
8	FDR filter (1%)	FDR threshold
9	Normalize	Normalization
10	Differential analysis (Perseus)	DAPs; ratio-compression handling; e-signature

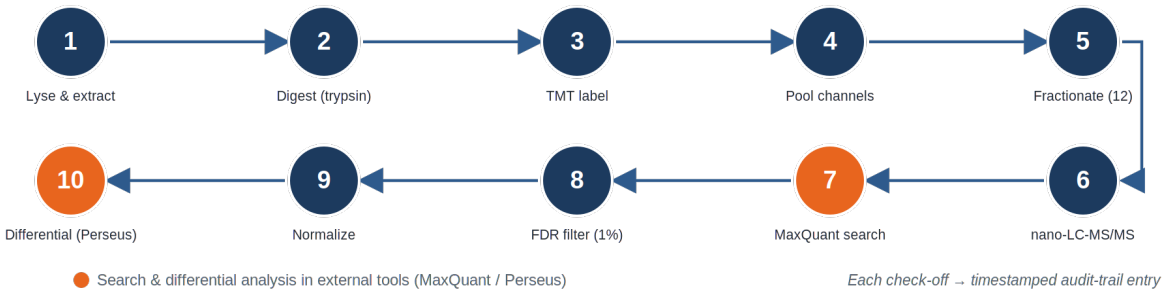

Figure 2. The 10-step bottom-up TMT workflow — orange steps are the search and differential analysis performed in external tools (MaxQuant / Perseus); every check-off writes a timestamped entry to the ELabELN audit trail.

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4. The Use Case: When and How the Template Is Used

The template is intended as a tested baseline for academic and biotechnology labs running quantitative proteomics and related mass-spectrometry workflows. It is configured around a recognizable reference — a bottom-up TMT 10-plex study on cell lysates — but the scenarios it serves span the proteomics bench and its downstream analysis.

4.1 Quantitative Proteomics (Primary Use Case)

The core scenario: measuring relative protein abundance across sample groups. The template captures the labeling scheme, the acquisition and search parameters, and the top differentially abundant proteins in one structured record, so a fold change is fully reconstructable — which channel, which parameters, which analysis — rather than a number in a spreadsheet detached from its design.

4.2 Post-Translational-Modification Mapping

PTM studies (phospho-, ubiquitin-, acetyl-proteomics) add an enrichment step and modification-specific search parameters. The template's typed fields extend to those parameters, keeping the enrichment and search settings on the same record as the acquisition.

4.3 Biomarker Discovery

Discovery cohorts compare many samples to find candidates. Because the labeling scheme and results are structured and queryable, candidates can be traced back to their exact channels and parameters, and compared across cohorts as the study scales.

4.4 Protein-Interaction Studies

Interaction workflows (AP-MS, proximity labeling) share the digest–label–acquire–search structure with different controls. The template documents the design and parameters that distinguish specific interactors from background.

4.5 Cross-Cohort and Multi-Batch QC

Because labeling schemes, parameters, and results are captured together, the template doubles as a running QC record across batches. A lab can pull every cohort run under a method version or TMT lot and compare identification depth, normalization, and differential results — the objective basis for detecting a batch effect before it confounds a conclusion.

4.6 Multi-Role Teams, Facilities, and CROs

Proteomics is inherently collaborative. Because every ELabELN edition includes unlimited users, the PI, sample-prep postdocs, MS facility staff, computational analysts, and rotating collaborators can all work from the same record. Granular permissions let the PI control who can edit sample prep versus the instrument method versus the search parameters — the role separation a core facility or CRO needs so each contributor owns their stage without overwriting another's.

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5. Dependencies and Connected Workflows

The MS template does not exist in isolation. It sits inside a network of connected workflows — upstream, parallel, external, and downstream — that give the run record its full scientific and provenance value.

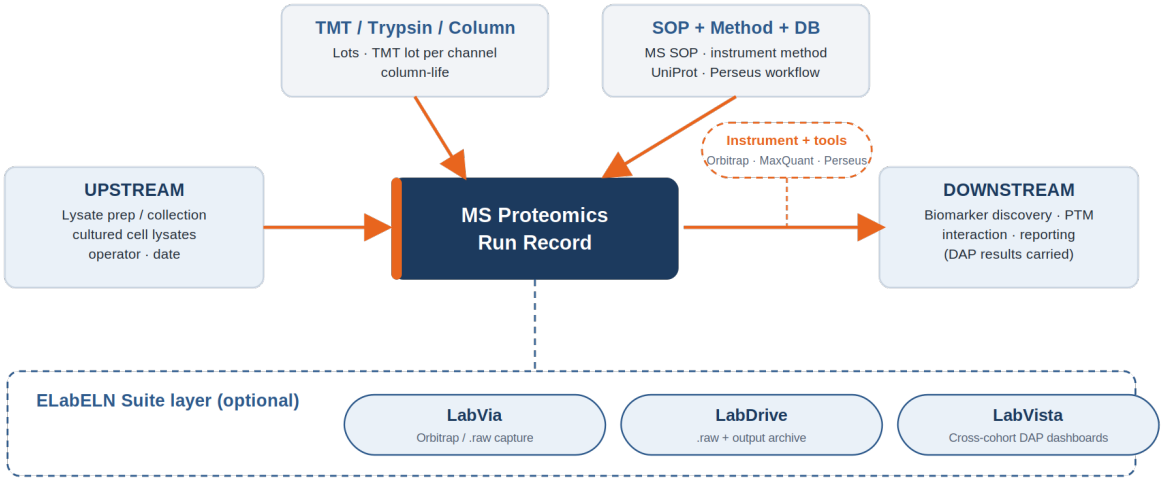

Figure 3. The template connects an upstream lysate prep, parallel inventory and SOP/method/database systems, the external instrument-and-software pipeline, and downstream discovery and reporting workflows.

5.1 Upstream: Lysate Preparation and Collection

Every run begins with prepared samples — cultured cell lysates, tissue, or another source. The template links to the upstream lysate-prep record, so opening a run surfaces the sample groups, the protein input, and the operator and date, anchoring every channel to the material behind it.

5.2 Parallel: TMT, Trypsin, and Column Inventory

The Compounds section links the TMT reagents, trypsin, the column, mobile phase, and reference digests directly to the ELabELN inventory. Because reagent lots and column condition drive quantitative comparability, this traceability is decisive. Through the link the record automatically carries:

- **The TMT lot shown inline with its channel**, so labeling provenance is tied to the exact reagent per channel.
- **Trypsin lot and column-life**, so a digest or separation issue can be traced to a reagent or an aging column.
- **Expiry and stock levels**, with low-stock warnings before a run, so a cohort is not started against a depleted or expired reagent.

Barcode and QR scanning can populate these links from the physical vial, keeping lot capture effortless across a long prep.

5.3 Parallel: SOPs, Instrument Method, Database, and Perseus Workflow

The Links section connects the run to the lab's version-controlled TMT 10-plex SOP (v2.1 by default), the instrument method file, the UniProt human reference database, and the Perseus workflow. Because these are version-controlled in ELabELN, every run records exactly which

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method, database, and analysis workflow it used — the anchors that cross-cohort comparison depends on.

5.4 External: The Instrument and Analysis Pipeline

The Orbitrap acquires the raw spectra, MaxQuant performs the database search and quantification, and Perseus performs the differential analysis. ELabELN is the system of record around that pipeline: the labeling scheme, instrument and LC parameters, search engine and database, and FDR threshold are captured as typed fields; the TMT labeling scheme (channel to sample) and the top differentially abundant proteins summary live in the spreadsheet editor; and the raw .raw files, the peptide.txt and proteinGroups.txt output, and the Perseus session files attach to the record. The design, the raw data, and the interpreted result stay together in one place.

5.5 Downstream: Discovery, Reporting, and Cross-Cohort Analysis

The differential-abundance results feed biomarker discovery, PTM interpretation, interaction mapping, and reporting, and — because the schemes, parameters, and results are typed and queryable — cross-cohort analysis across a shared proteomic resource. A batch effect or a drifting reagent shows up when cohorts are compared, not after a conclusion is drawn.

5.6 The ELabELN Suite: Instruments and Dashboards

Everything above is available in ELabELN Standard. Labs on the ELabELN Suite gain three layers that connect to the same record: LabVia captures acquisition data directly from the Orbitrap; LabDrive adds metadata search, versioning, and role-based access across .raw and output-file archives; and LabVista builds cross-cohort differential-abundance dashboards on the structured labeling and result metadata. The same audit trail and data-integrity controls span all layers.

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6. How the Team Benefits

The template is built to deliver value at every stage of the pipeline, not just at the bench. The benefits compound with every cohort a lab runs.

6.1 Start From a Tested Baseline, Not a Restated Method

The scaffold — protocol, typed fields, reagent links, SOP, instrument method, database, and analysis workflow — is already built. The team edits a working configuration to match the study they actually run, rather than restating the method from scratch every cohort. The first run is faster, and every subsequent one is consistent with it.

6.2 Document by Doing, Across Every Stage

Checking off each of the 10 steps as it happens produces a contemporaneous, timestamped record as a by-product of the work, and the instrument run is auto-logged. Sample prep, acquisition, and analysis are documented as they occur, by whoever performs them — with no separate write-up to reconstruct later.

6.3 Never Lose the Labeling Scheme or Lot Provenance Again

Because the channel-to-sample assignment is a structured field and the reagents are linked to inventory, the labeling scheme, TMT lot per channel, trypsin lot, and column-life are captured permanently on every run. When a fold change is questioned, the scheme and provenance are on the record — closing the most consequential proteomics gap by default.

6.4 Cross-Cohort Comparisons You Can Query

Typed labeling, parameter, and result fields make the study queryable. A team can pull every cohort run under a method version or TMT lot, compare identification depth and differential results, and catch a batch effect early — instead of discovering it after the study is assembled.

6.5 Audit-Ready Records with Role Separation

The tamper-evident audit trail, version-controlled linkage, electronic signatures, and granular permissions mean the record that results from normal use is already structured to support cross-cohort reproducibility documentation, multi-PI collaboration on shared proteomic resources, and FDA 21 CFR Part 11 review when the lab's quality system requires it — with each contributor owning their stage of the record.

> **AT THE BENCH, IN PRACTICE**
>
> A postdoc opens the template, enters the TMT channel-to-sample assignment as a structured table, scans the TMT and trypsin vials to capture their lots, and checks off lysis and digest. The facility scientist records the instrument method and acquisition parameters as the Orbitrap run auto-logs. The computational analyst records the MaxQuant database and FDR, notes that SPS-MS3 was used so ratio compression is bounded, and attaches the Perseus session with the top differentially abundant proteins. Months later, comparing cohorts, the PI queries every run on that TMT lot and sees whether the depth and ratios held.

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7. The Labeling Scheme and Differential Abundance

7.1 The Default Reference: A TMT 10-Plex Study

The template ships configured for a bottom-up TMT 10-plex study: ten samples — five control and five treated in the reference design — each labeled with a distinct isobaric tag, pooled, fractionated into 12 high-pH reverse-phase fractions, and analyzed in separate 90-minute nano-LC-MS/MS runs on an Orbitrap with HCD fragmentation. After the MaxQuant search and FDR control, normalization and a Perseus differential-abundance test produce the up- and down-regulated proteins between groups. This concrete reference demonstrates the full design-to-result workflow out of the box; swap the labeling scheme, instrument, or analysis pipeline to match what your lab runs.

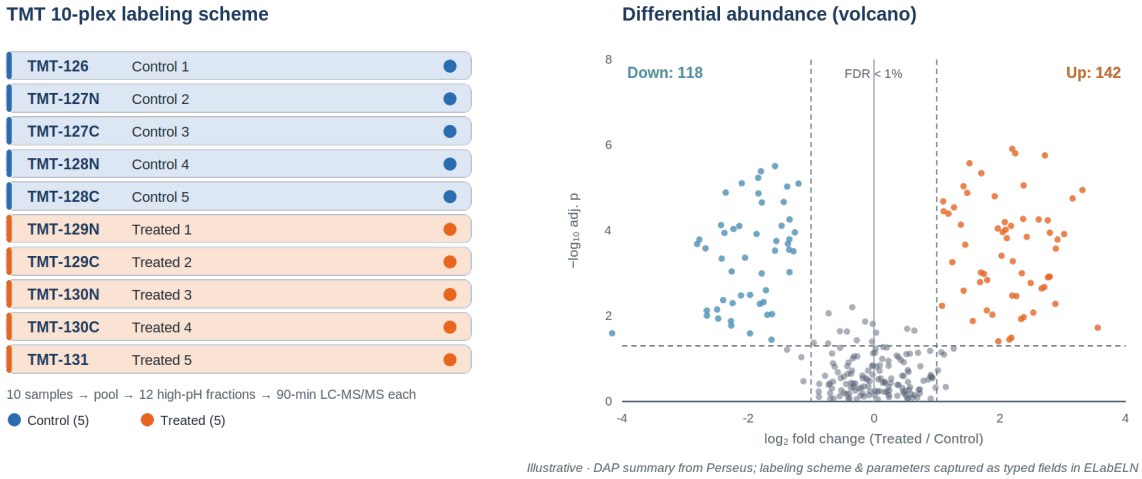
TMT 10-plex labeling scheme
TMT-126 Control 1
TMT-127N Control 2
TMT-127C Control 3
TMT-128N Control 4
TMT-128C Control 5
TMT-129N Treated 1
TMT-129C Treated 2
TMT-130N Treated 3
TMT-130C Treated 4
TMT-131 Treated 5
10 samples → pool → 12 high-pH fractions → 90-min LC-MS/MS each
Control (5)
Treated (5)
Differential abundance (volcano)
Down: 118
FDR < 1%
Up: 142
−log10 adj. p
log2 fold change (Treated / Control)
Illustrative · DAP summary from Perseus; labeling scheme & parameters captured as typed fields in ELabELN

Figure 4. The TMT 10-plex channel-to-sample assignment alongside a differential-abundance volcano plot of the resulting up- and down-regulated proteins. Illustrative; the differential-abundance summary comes from Perseus, and the labeling scheme and parameters are captured as typed fields in ELabELN.

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7.2 How the Template Handles the Scheme, Parameters, and Results

8. Configuring the Template for Your Workflow

Adapting the template to a different scheme or instrument is a matter of editing the relevant sections — not rebuilding the structure.

8.1 Swap the Labeling Scheme

Change the labeling scheme — label-free, SILAC, TMT-6plex, TMT-10plex, TMT-16plex, or TMT-Pro — by editing the labeling section and the channel-to-sample table. If the reagents already exist in the ELabELN compound database, simply re-link them; their lots flow in with the channel.

8.2 Change the Instrument and Acquisition Mode

Switch the instrument (Q Exactive, Orbitrap Exploris, Orbitrap Astral, timsTOF Pro, timsTOF SCP, Stellar) and the acquisition mode (DDA, DIA, BoxCar, PRM, SureQuant) to match your platform. The instrument and resolution fields apply across all of them.

8.3 Change the Search Pipeline, and Bottom-Up vs. Top-Down

Change the search engine and database (MaxQuant, FragPipe, Proteome Discoverer, Sage), or move from bottom-up to top-down by editing the digest and search sections. The FDR and result-filtering fields work the same way.

8.4 Save a Custom Version

Once configured, save your edits as a private template scoped to your lab, or publish back to the ELabELN template library. Every subsequent cohort opens from your configured, version-controlled method, and separate versions can be maintained for different schemes, instruments, or study types.

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9. Getting Started

ELabELN Standard is a cloud-hosted SaaS deployment typically live within one to two business days of account creation. There is no hardware to buy, no IT project, and no per-seat licensing.

1. **Start an ELabELN account.** Visit elabeln.com/get-started. ELabELN Standard runs on LabLynx's managed cloud infrastructure.
2. **Provision your instance.** LabLynx provisions the instance within one to two business days; you receive a URL, admin credentials, and onboarding documentation.
3. **Load the mass spectrometry template.** From the template library, select the mass spectrometry template and click “Use This Template.” An editable instance opens immediately.
4. **Add your reagents and columns to the inventory.** Enter your TMT reagents, trypsin, columns, mobile phase, and reference digests with lot numbers, column-life, and −80 °C storage locations. This is a one-time setup step.
5. **Link your SOP, method, database, and Perseus workflow.** Upload your MS SOP and instrument method, and connect them, along with the search database and Perseus workflow, to the template's Links section.
6. **Customize the template for your study.** Edit the labeling scheme, channel assignment, instrument and acquisition mode, and search pipeline, then save as a private team version.
7. **Run your first cohort.** Open your saved template, complete the 10-step checklist across sample prep, acquisition, and analysis, attach the .raw and output files, and have the PI sign off electronically.

TYPICAL TIMELINE

Day 1: Account requested at elabeln.com/get-started. Day 2–3: Instance provisioned; reagent/column inventory populated; SOP, method, database, and Perseus workflow linked. Day 3–4: Template configured and saved as a private version for your study design. Day 4–5: First cohort documented in ELabELN with the labeling scheme, parameters, and differential results captured and an e-signature.

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9.1 ELabELN Standard vs. ELabELN Suite

Capability	Standard	Suite
Mass spectrometry template access	Included	Included
Unlimited users	Included	Included
Audit trail and e-signatures	Included	Included
TMT / trypsin / column inventory with lot & column-life	Included	Included
SOP, method, database & Perseus workflow linking	Included	Included
.raw, output & Perseus session attachments	Included	Included
LabVia direct Orbitrap / .raw capture	—	Suite layer
LabDrive .raw + output archive search & versioning	—	Suite layer
LabVista cross-cohort differential-abundance dashboards	—	Suite layer

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10. Frequently Asked Questions

Can I configure the template for my labeling scheme and instrument?

Yes. Every section is editable. Swap in different labeling schemes (label-free, SILAC, TMT-6plex, TMT-10plex, TMT-16plex, TMT-Pro), change the instrument (Q Exactive, Orbitrap Exploris, Orbitrap Astral, timsTOF Pro, timsTOF SCP, Stellar), adjust the acquisition mode (DDA, DIA, BoxCar, PRM, SureQuant), or change the search engine and database. Save your edits as a private template scoped to your lab, or publish back to the ELabELN template library.

Does the template work for metabolomics or lipidomics too?

This template is configured for bottom-up proteomics. The structural pattern — sample prep, LC method, MS acquisition, identification, quantification — carries over to metabolomics and lipidomics, but the specific fields, library references (HMDB, LipidMaps), and analysis tools (MS-DIAL, XCMS, MetaboAnalyst, LipidSearch) differ enough that a dedicated template is more useful. The ELabELN team can scaffold a small-molecule MS variant during onboarding.

How does the template handle TMT ratio compression?

TMT ratio compression — the underestimation of fold changes caused by co-isolated interfering precursors — is a known issue with TMT quantification. The template captures whether SPS-MS3 quantification was used, or whether a ratio-compression correction was applied at the analysis level (for example via Perseus or MS-EmpiRe). The structured field means downstream interpretation of fold-change values carries the appropriate caveat, documented in the experiment record.

Is it included in every ELabELN plan?

Yes. Every published template in the ELabELN library is available to all subscribers in both the Standard and Suite editions, with unlimited users in either edition and no per-template fee.

Can my whole lab use this template?

Yes. Every ELabELN edition includes unlimited users, so the PI, sample-prep postdocs, MS facility staff, computational analysts, and rotating collaborators can all use the template without per-seat charges. Granular permissions let the PI control who can edit sample prep versus the instrument method versus the search parameters.

How quickly can my lab start running proteomics in ELabELN?

ELabELN Standard cloud deployment is typically live in one to two business days. Once the instance is provisioned, the template loads from the library in a single click, with the labeling scheme, instrument method, and analysis pipeline editable to match the proteomics workflows your lab actually runs.

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11. Conclusion

The ELabELN Mass Spectrometry Experiment Template is not simply a digital version of a proteomics worksheet. It is a structured, audit-ready, searchable record that connects to your reagent and column inventory, your SOPs, instrument method, and search database, the lysates the study measured, your instrument and analysis pipeline, and the discovery and reporting the results feed — and, in the Suite edition, cross-cohort differential-abundance dashboards. It turns a workflow that spans many hands and several tools into a single record whose labeling scheme, parameters, and results are captured, comparable, and defensible.

For a laboratory that runs proteomics regularly, the benefit compounds with every cohort. Labeling schemes, acquisition and search parameters, and differential results accumulate into one queryable, cross-cohort history. Every TMT lot and column is traceable. Every method version is documented. Every stage is timestamped and attributed to whoever performed it — so a lost labeling scheme or an undocumented parameter can no longer break a study, and a batch effect is caught before it confounds a conclusion.

The template is available to all ELabELN subscribers today. A new instance is live in one to two business days, and the first structured cohort is typically documented within a week of account creation.

GET STARTED

Visit elabeln.com/get-started to request your ELabELN instance, or contact LabLynx at 866.522.5969 or info@lablynx.com. Load the mass spectrometry template, configure it for your labeling scheme and instrument, and run your next cohort from a tested, audit-ready baseline.

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